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Measurement of properties and pilot testing. CERE lab and model development

Fosbøl, Philip Loldrup

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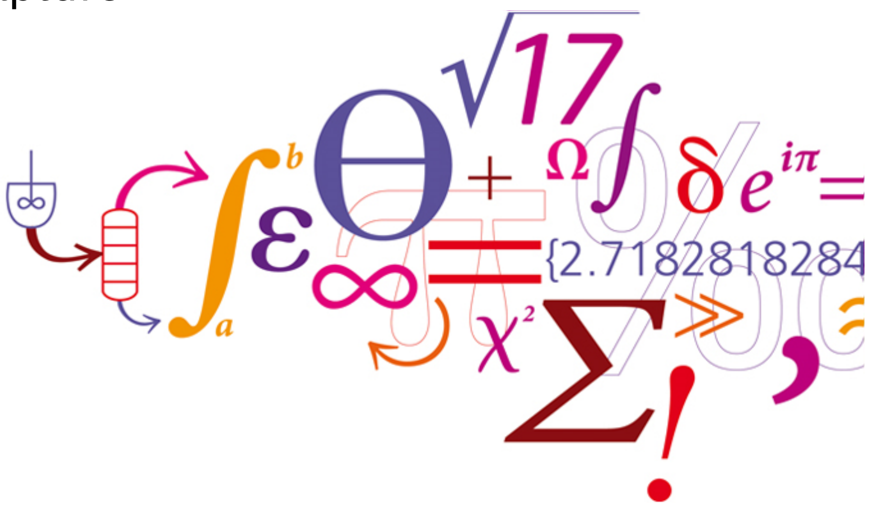
Measurement of properties and pilot testing

CERE lab and model development

Application: Rate based modeling of CO_2 capture



Philip Loldrup Fosbøl

+ many students and faculty

EFCE WP, May 12th 2016

CERE
Center for Energy Resources Engineering

DTU Chemical Engineering
Department of Chemical and Biochemical Engineering

CERE Industrial Consortium 2016

DTU

calsep

AkzoNobel

bp

Chevron

DONG energy

ConocoPhillips

Eni

GASSCO

Genel Energy International

ExxonMobil

Linde Engineering Linde

GASSNOVA

HESS

INFOCHEM

ifp

GDF SUEZ

NOV NATIONAL OILWELL VARCO

RWE The energy to lead

Lloyd's Register Consulting

BR

OMV

Sinopec

Statoil

SQM THE WORLDWIDE BUSINESS FORMULA

Schlumberger

UNION ENGINEERING Reliable solutions by dedicated people

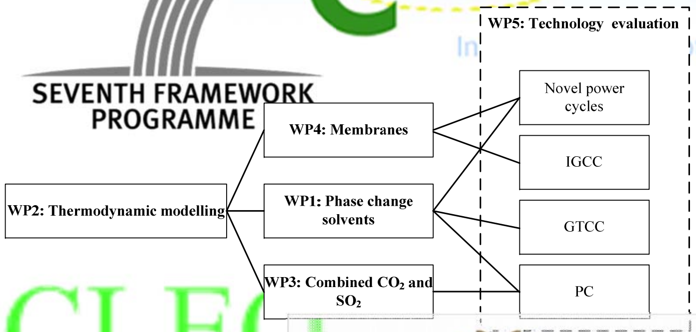
MAERSK OIL

Welltec®

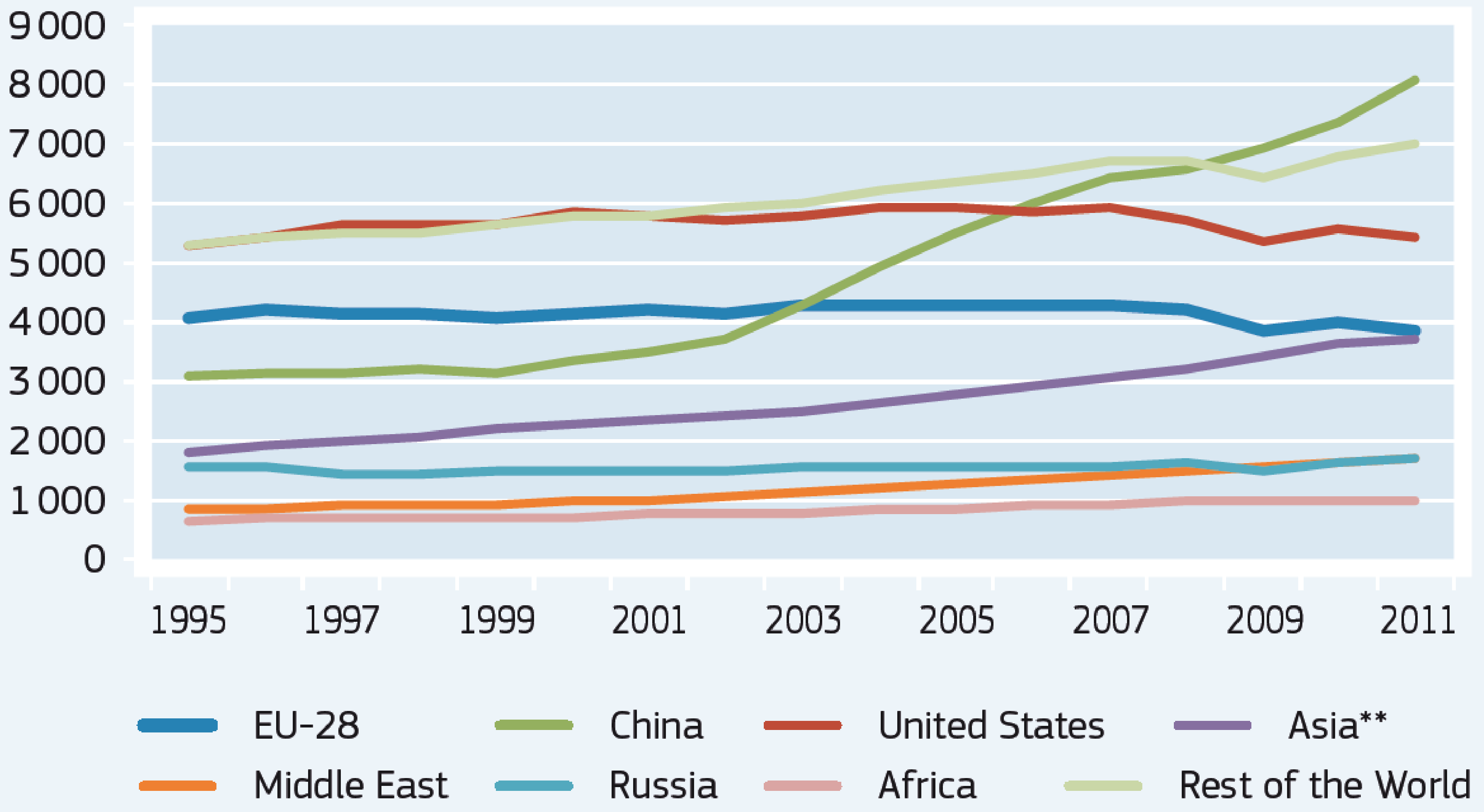
TOTAL

EU Activities

- CASTOR
  - FP6 EU project
- iCap
  - Gas hydrate
  - Demixing process
- CESAR/CLEO
  - Thermodynamic model implementation
  - CASTOR comparison
- OCTAVIUS
  - Process Benchmarking
  - CAPE-Open develoment
- INTERACT
  - Lab scale & pilot trials using enzymes
- EERA
  - Preparation of consortia idea creation for new EU calls



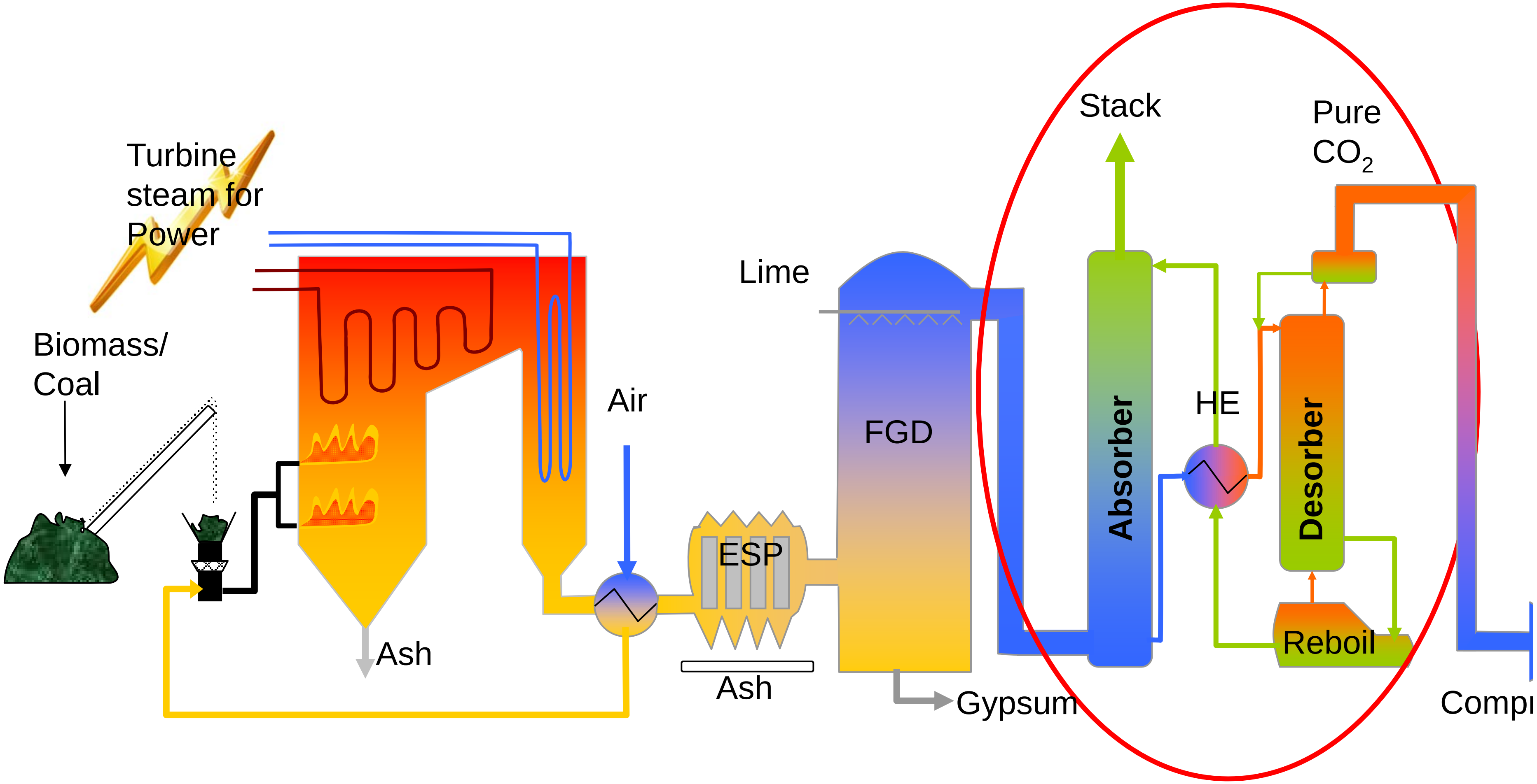
World CO_2 Emissions by Region (Mio ton CO_2)



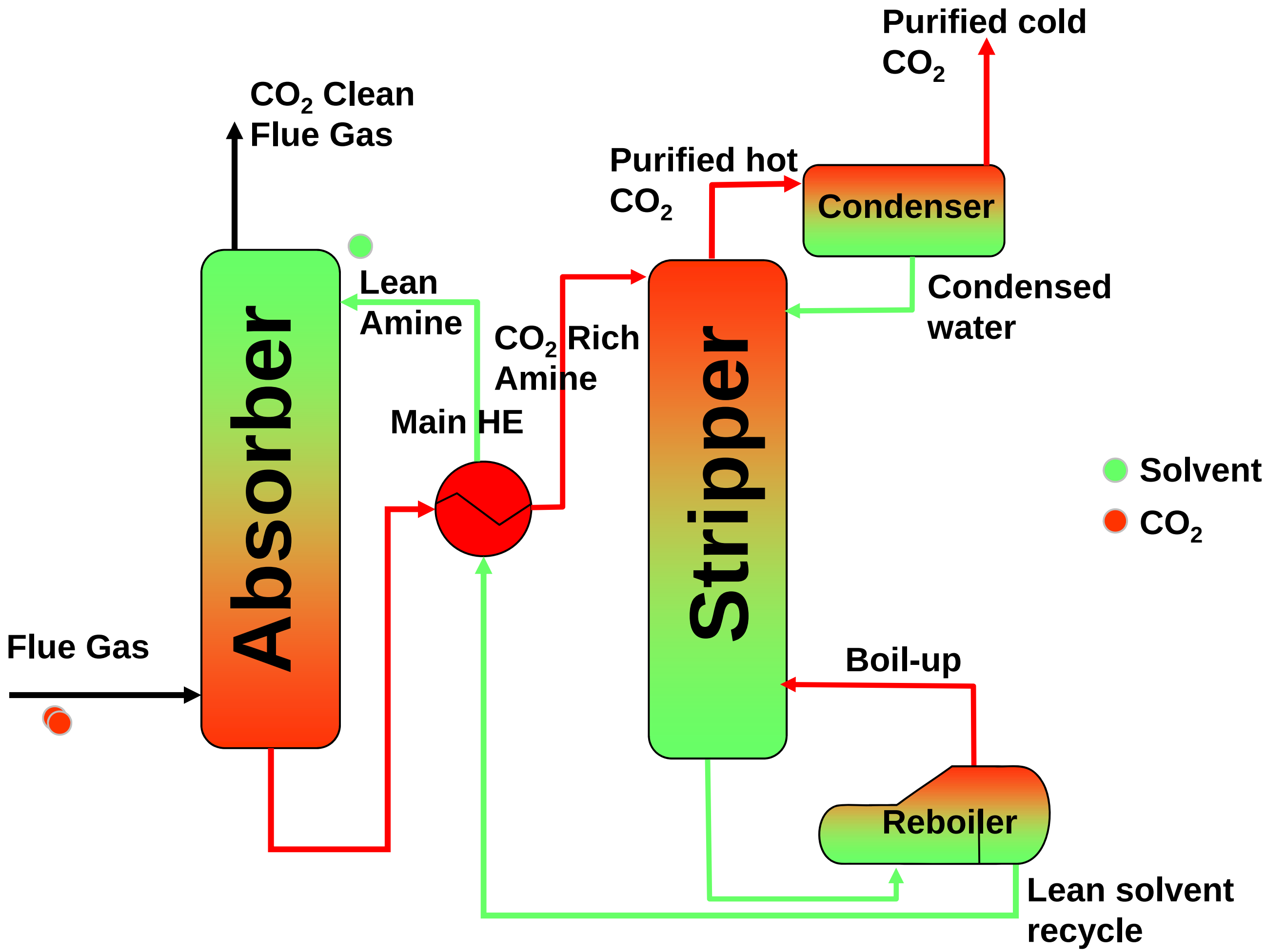
EU energy in figures 2014

Australian “Coal Mountain”

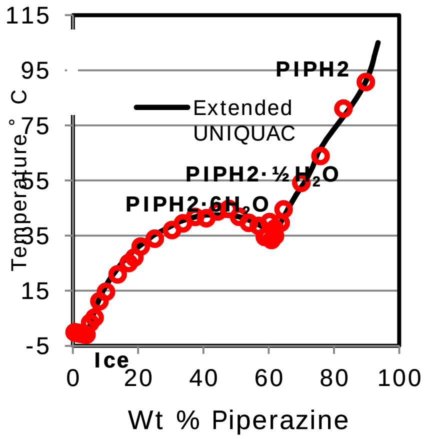
Carbon capture and storage (CCS)



CO_2 capture



Purified cold CO2
CO2 Clean Flue Gas
Purified hot CO2
Condenser
Lean Amine
Condensed water
CO2 Rich Amine
Absorber
Stripper
Main HE
Solvent
CO2
Flue Gas
Boil-up
Reboiler
Lean solvent recycle

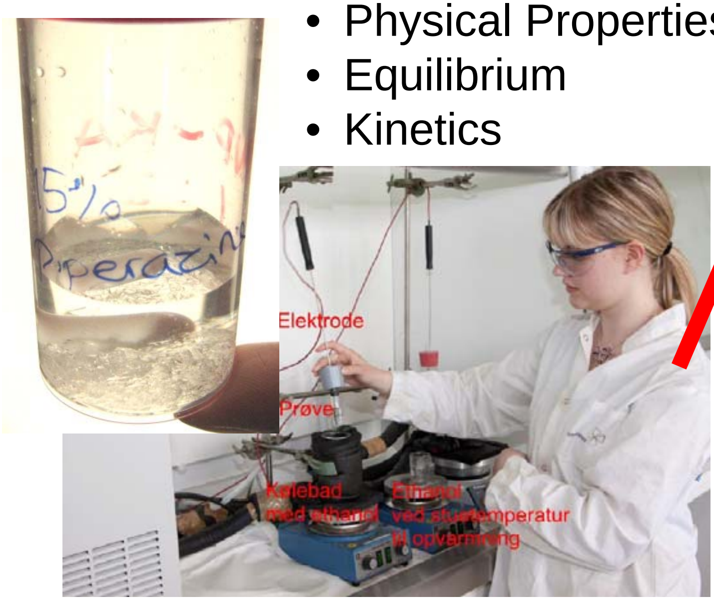


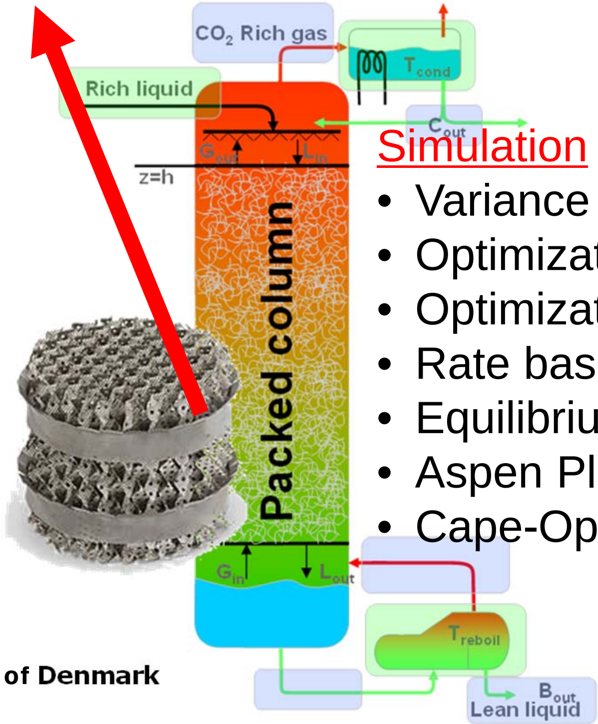
Modelling
- Energy consumption
- Heat of reaction
- Thermodynamics
- Kinetics

Pilot tests
- Real life tests
- Solvent study
- Packing testing
- Energy requirements
- Mass transfer

Emission CO_2 reduction

Experimental
- Physical Properties
- Equilibrium
- Kinetics





Simulation
- Variance analysis
- Optimization of energy use
- Optimization of packing
- Rate based approach
- Equilibrium approach
- Aspen Plus
- Cape-Open

CO LaN

Rate based model (CapCO$_2$)

- Gas balance

Total: $\frac{dG}{dz} = -\left(N_C + N_W\right)aS$

CO_2: $G\frac{dy_C}{dz} = -y_C\frac{dG}{dz} - N_C aS$

H_2O: $G\frac{dy_W}{dz} = -y_W\frac{dG}{dz} - N_W aS$

Energy: $GC^G_{p,tot}\frac{dT_G}{dz} = -\left(\frac{dG}{dz}C^G_{p,tot} + aS\left(C^G_{p,W}N_W + C^G_{p,C}N_C\right)\right)T_G - qaS$

- Liquid balance

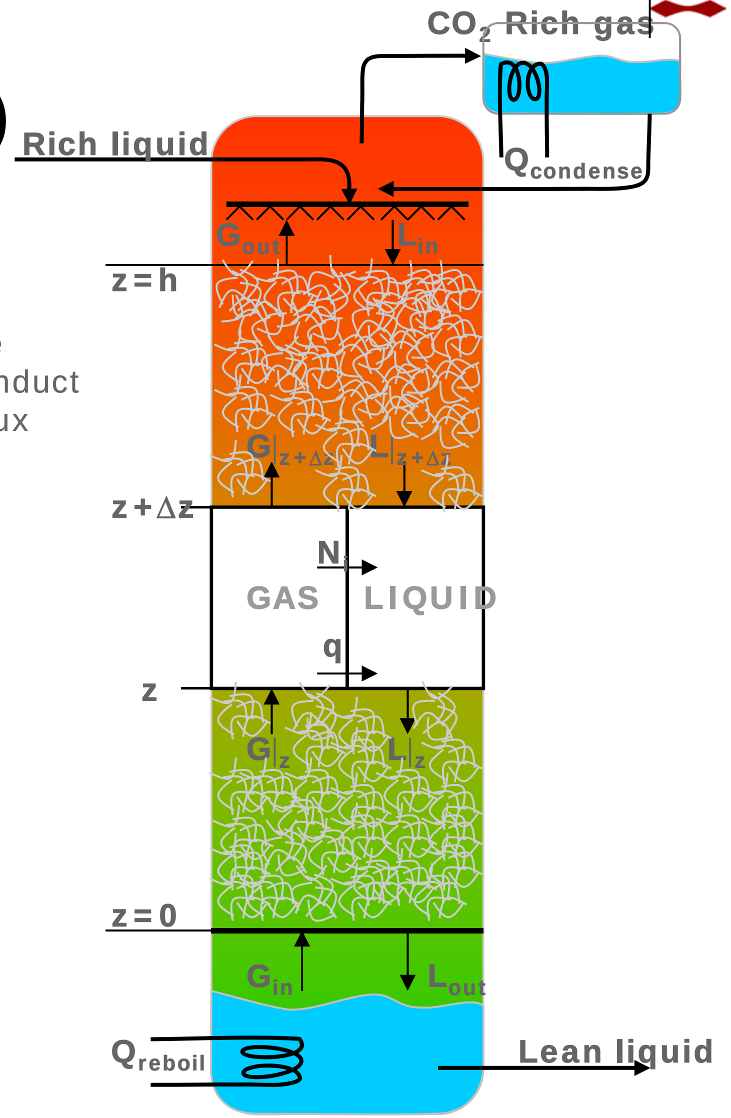
Total: $\frac{dL}{dz} = -N_W aS$

CO_2: $L\frac{dx_C}{dz} = -x_C\frac{dL}{dz} - N_C aS$

H_2O: $L\frac{dx_W}{dz} = -x_W\frac{dL}{dz} - N_W aS + N_C aS$

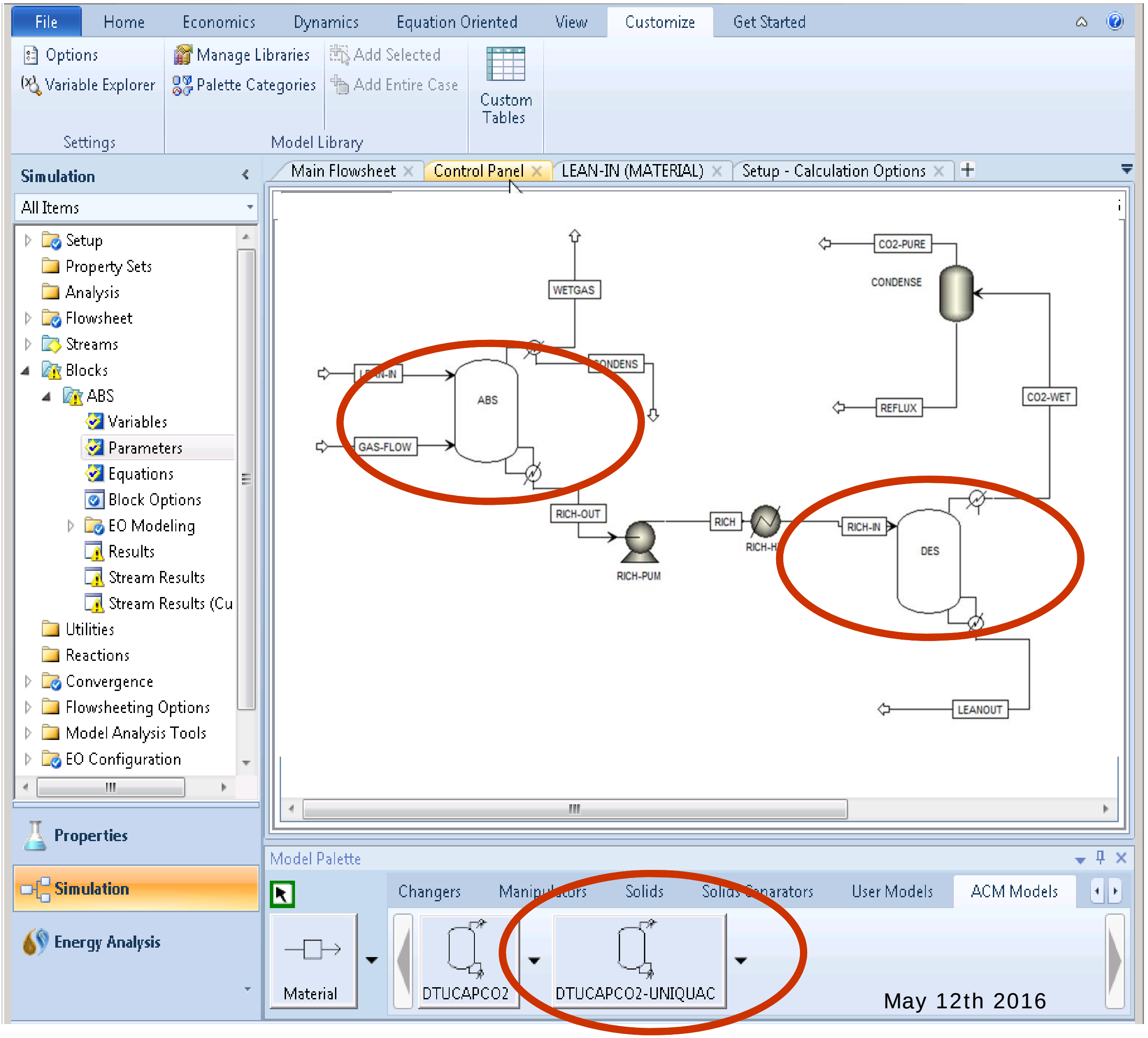
Energy: $C^L_{p,tot}L\frac{dT_L}{dz} = -C^L_{p,tot}T_L\frac{dL}{dz} - aS\left(\left(C^L_{p,W}T_G + \Delta_{vap}H_W\left(T_L\right)\right)N_W + \left(C^L_{p,C}T_G + \Delta_{CO_2,diss}H\left(T_L\right)\right)N_C\right) - qaS$

W: H_2O
C: CO_2
G: Gas
L: Liquid
z: Distance
q: Heat conduct
N: Mass Flux



CAPCO2 unit operation

Aspen Plus



Physical properties in Rate based modelling

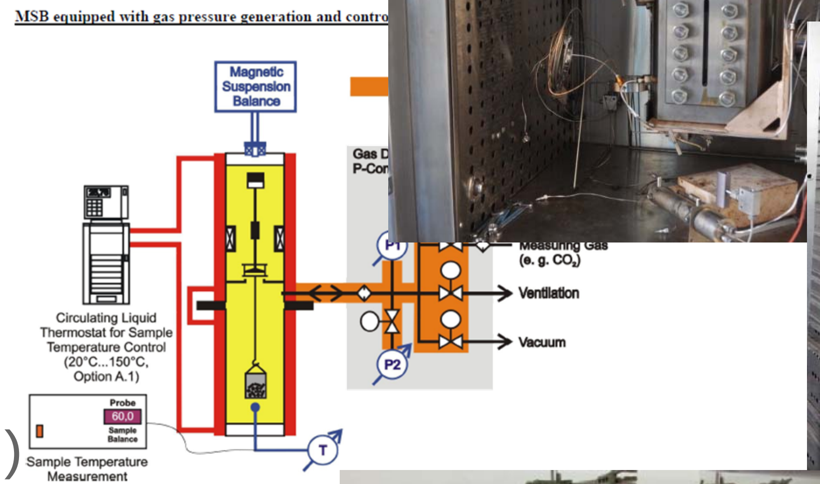
- Liquid properties
  - Diff. coef. A in W
  - Diff. coef. CO_2 in A-W sol.
  - Surface tension of W and A-W sol.
  - Viscosity of A-W sol.
  - Second order rate constant of CO_2 abs. in A-W
  - Thermodynamic properties
    - Heat cap. of solution
    - Henry's constant of CO_2 in A-W sol.
    - Equilibrium CO_2 pressure over A-W sol.
    - Heat of abs. of CO_2 in A-W sol.
    - Saturation pressure of W
    - Heat of vaporization of W
    - Density of pure W, A, and sol.

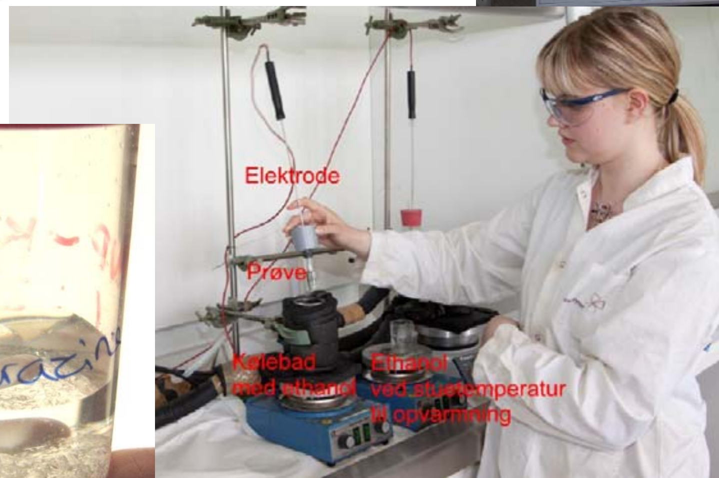
- Gas properties
  - Diffusivity of CO_2 in gas
  - Diffusivity of W in gas
  - Viscosity of gas (CO_2-Air-W)
  - Thermodynamic properties
    - Density of gas
    - Heat cap. of gas (CO_2, Air, W)

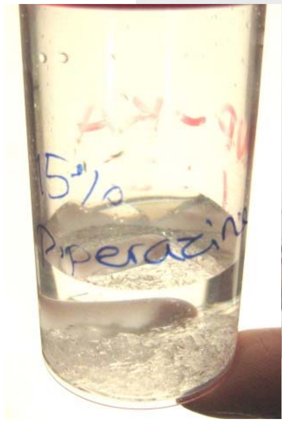
W: Water
A: Amine
Sol.: Mixture

Phase eq. & properties

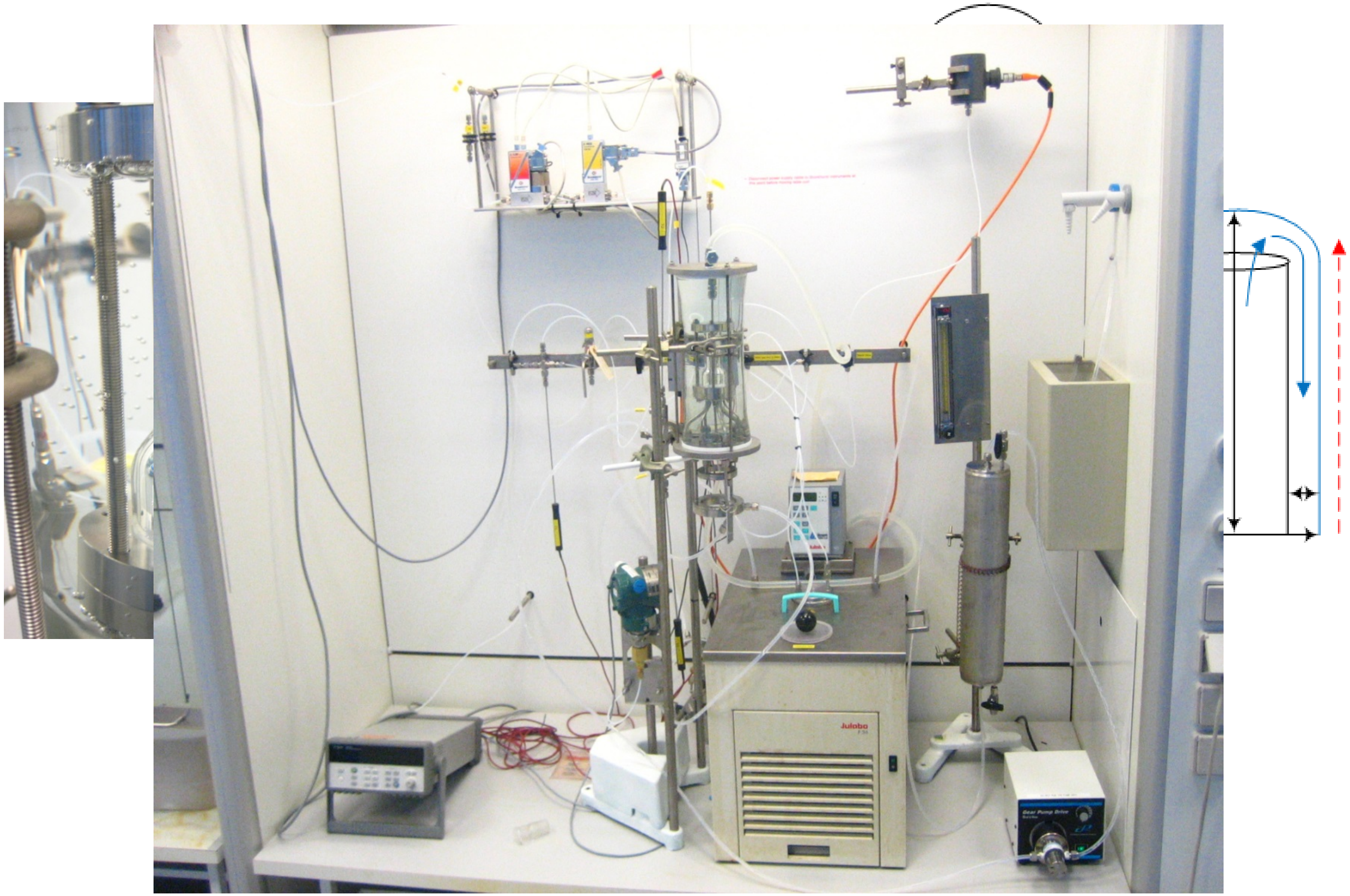
- CO_2 solubility
    - VLE
    - High P and T
- Slurry formation(SLE)
    - Freezing point depression
    - Solubility measurement
- Density
- Viscosity
- Surface tension



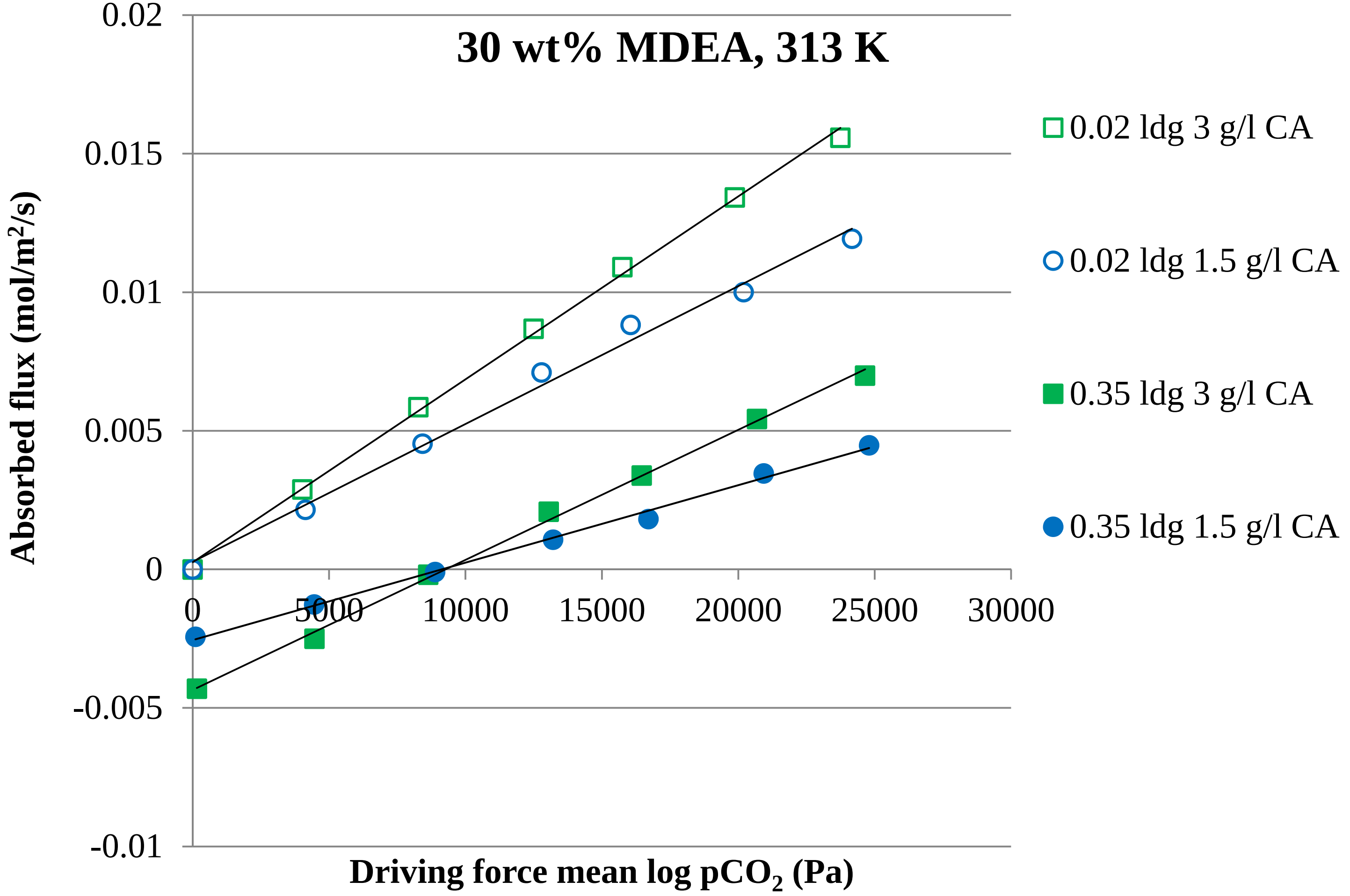




Reaction kinetics between CO_2 and solvent

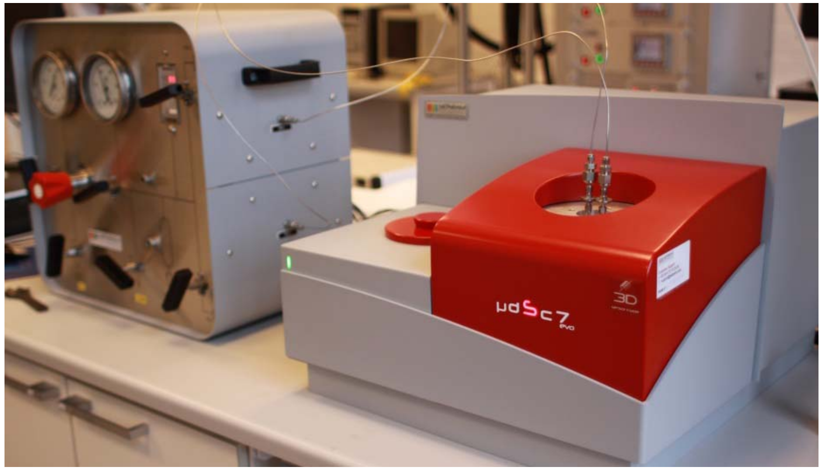


Kinetic result

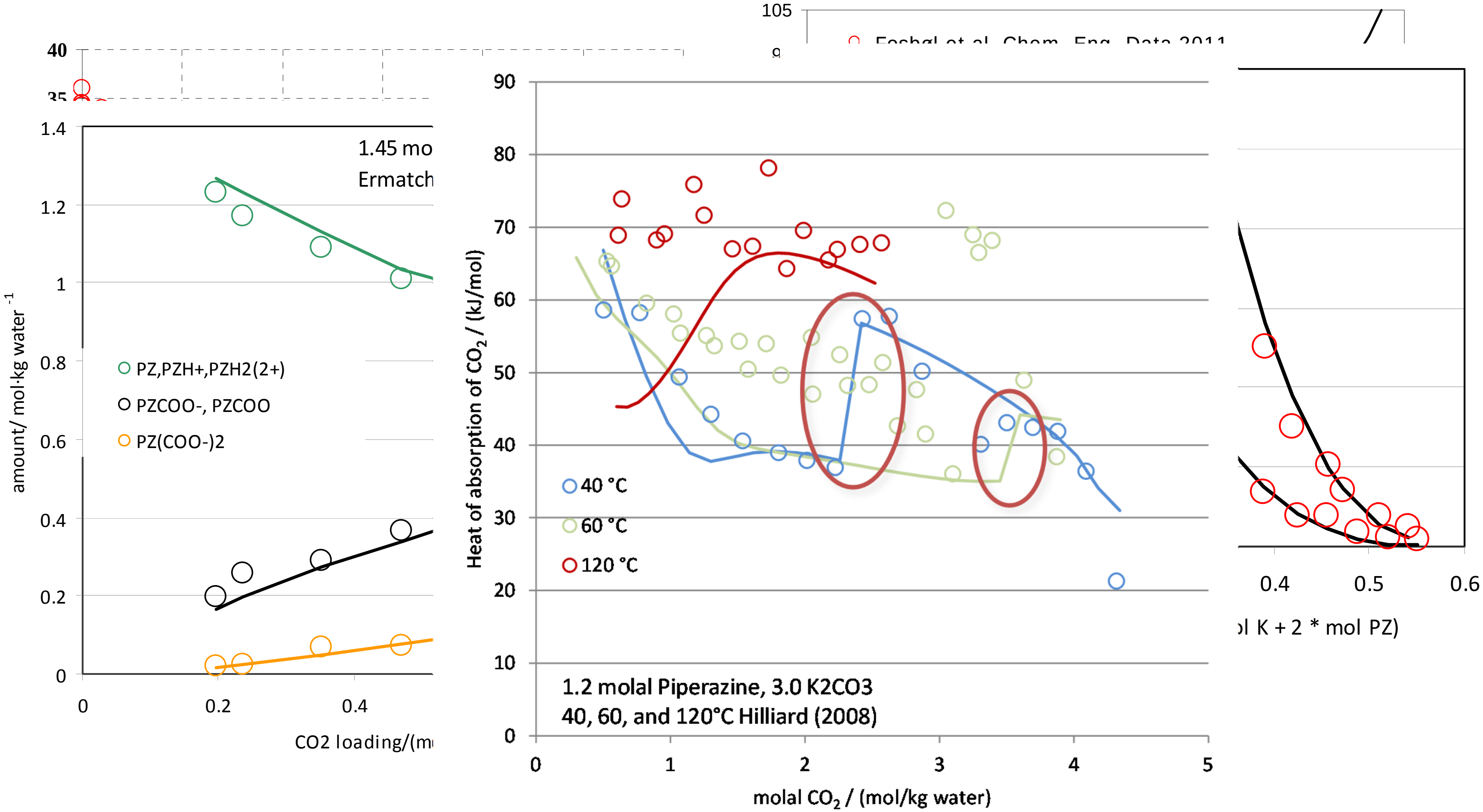


Experimental work - calorimetric

- High pressure DSC
- Phase change, heat of absorption by DSC



Thermodynamic modelling
ex: CO_2-PZ-K_2CO_3-$KHCO_3$-H_2O



Pilot tests and demonstration

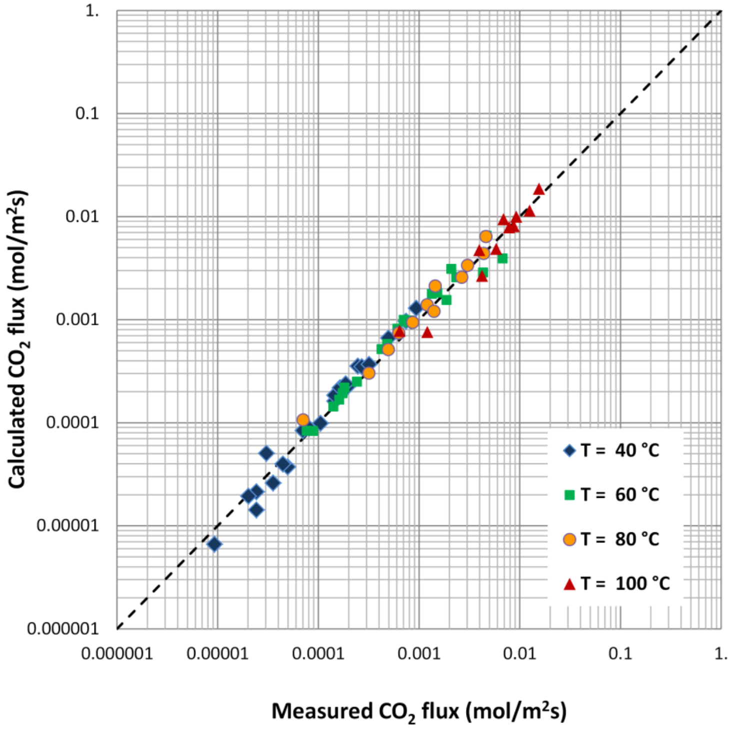
- CO_2 Absorber
  - 10m height (Variable height)
  - 10cm diameter
  - Capacity: Approximately 40Nm^3/h
  - Structured packing (Mellapack)
  - Temperature and sampling readings
    - Every meter
    - Temperature and loading profiles
  - Well developed DAQ for flow etc.

- Absorber test runs
  - Standard Amines
  - Enzymes

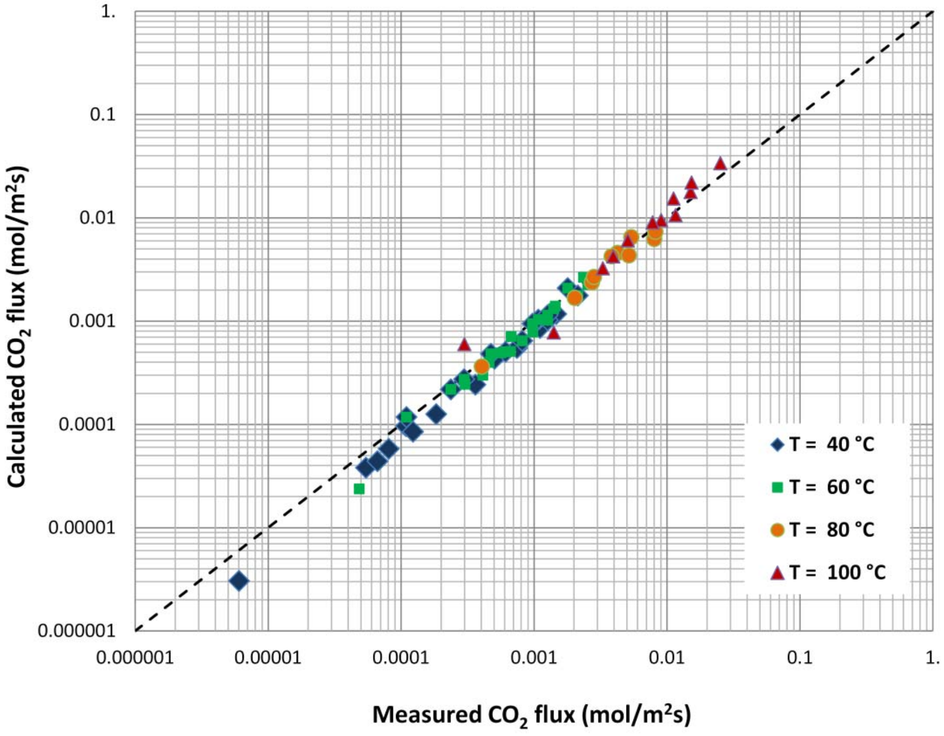
- Desorber
  - Design in progress

Mass Transfer Modeling

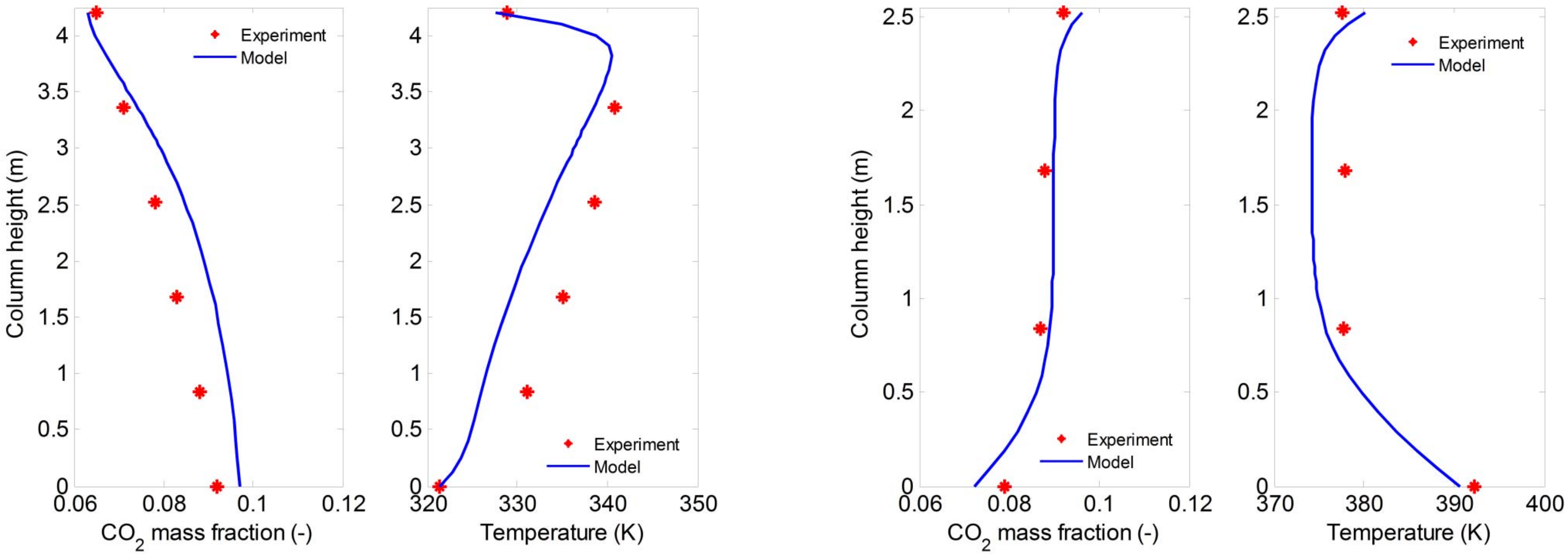
30 wt.% MEA



5 molal PZ

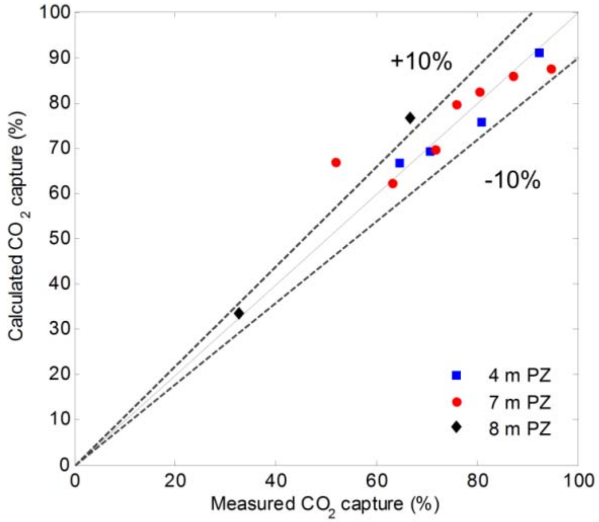


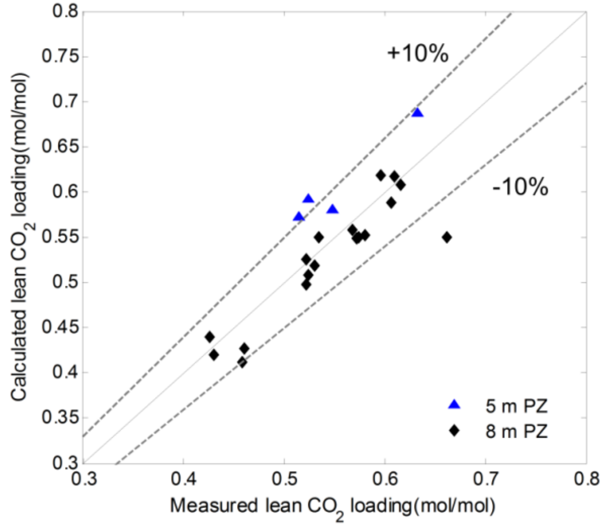
Comparison to pilot data

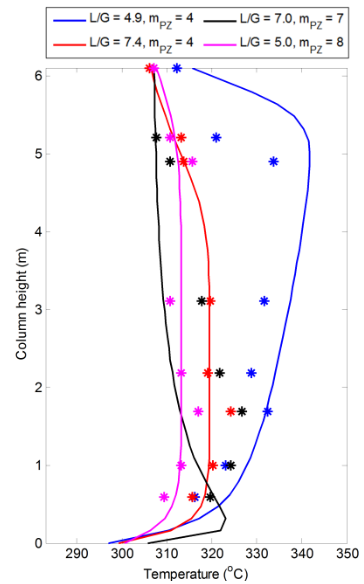


Modeling Innovative Solvents

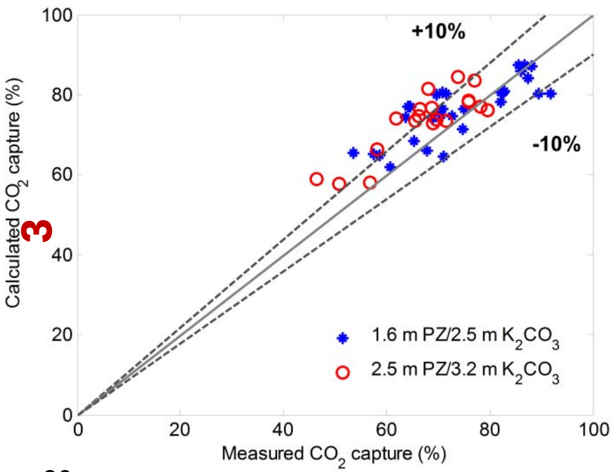
PZ

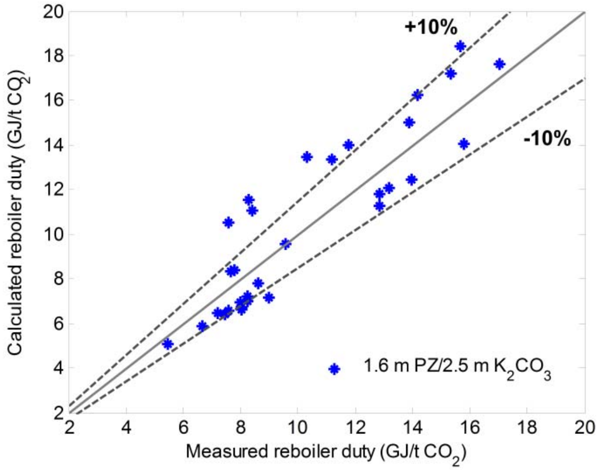


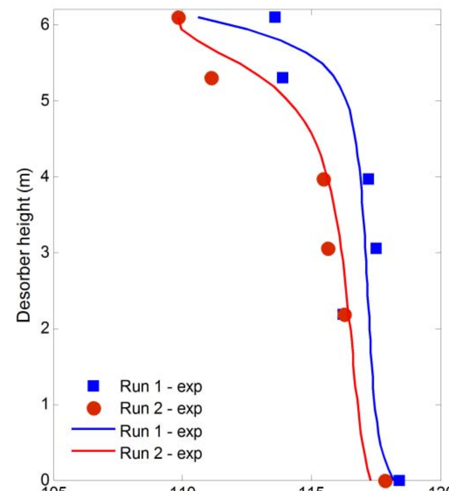




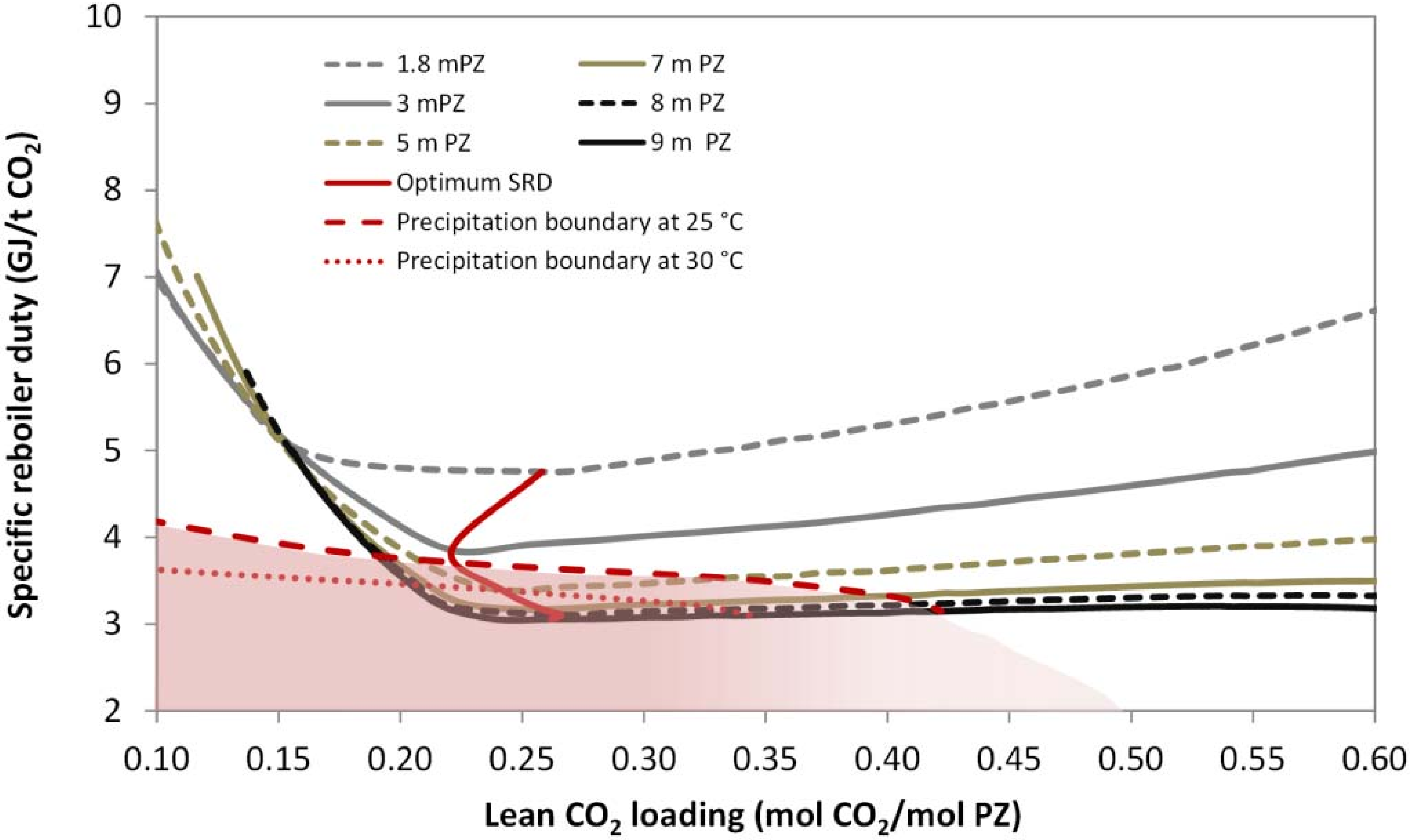
PZ+K_2CO_3





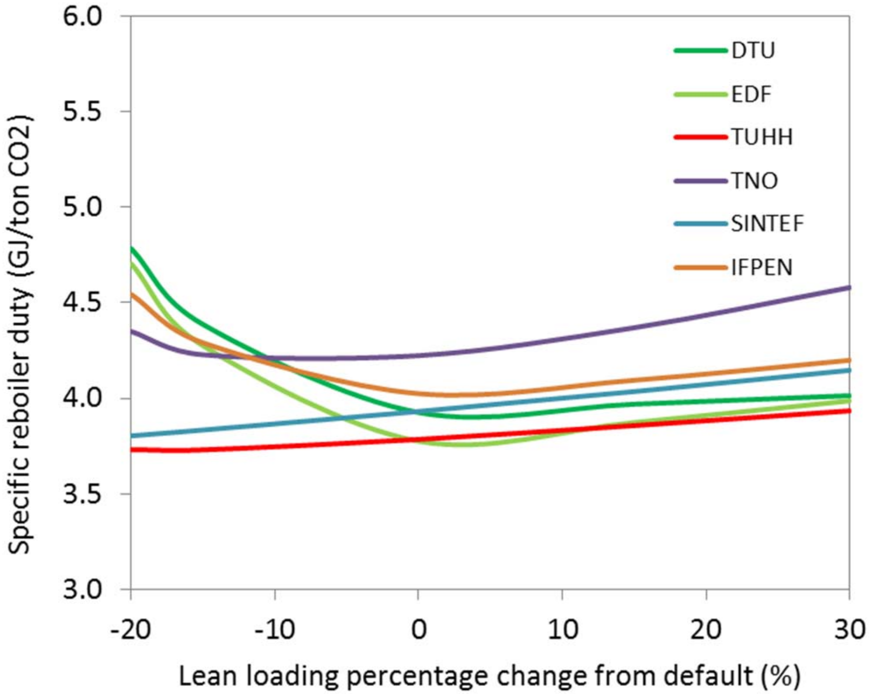


Rate based simulation with solids (PZ)

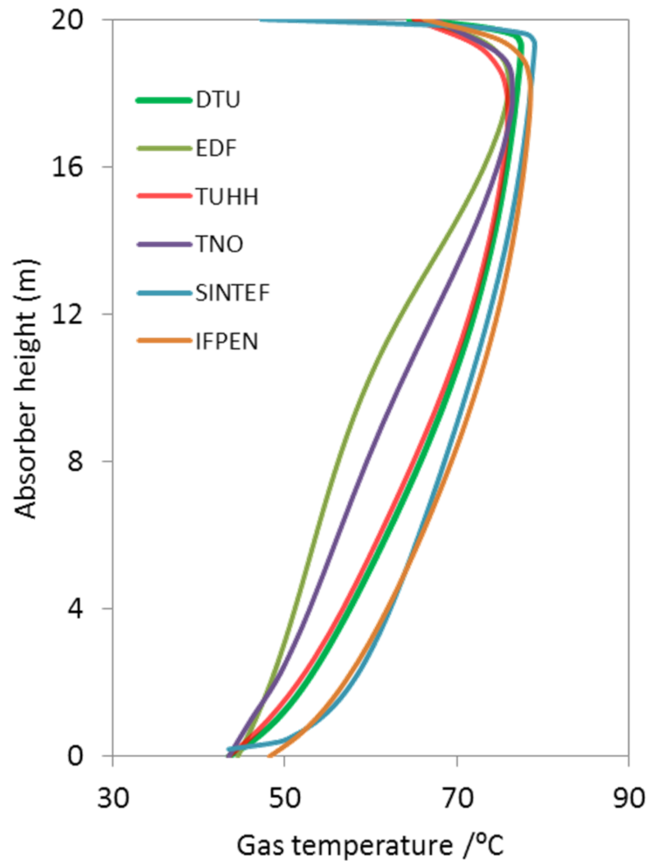


EU benchmarking

- Desorber reboiler duty
  - Good reproducibility (±5%)
  - High scatter at high flooding

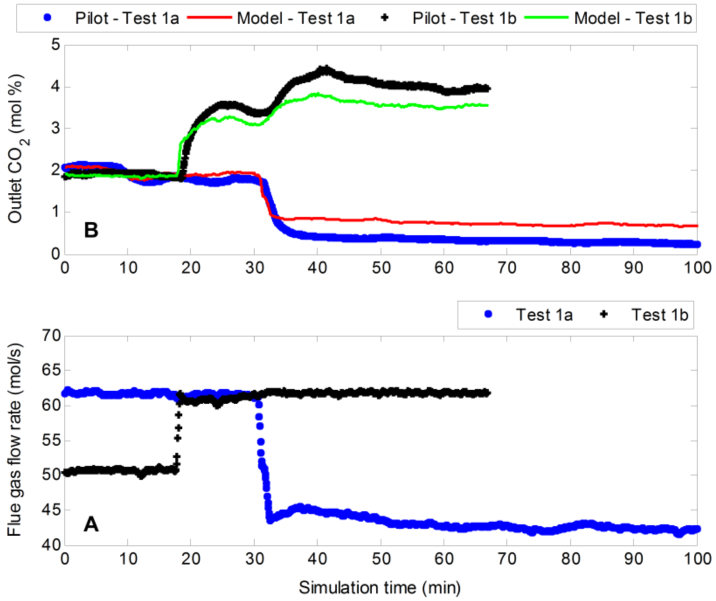


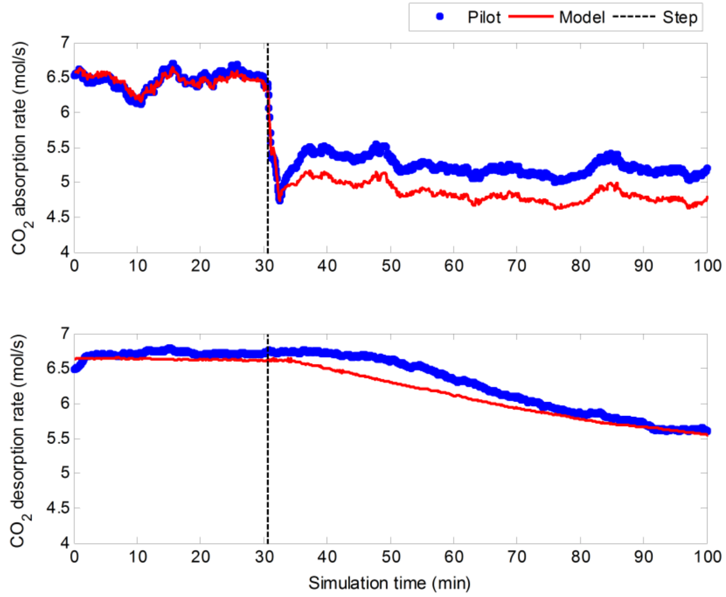
- Absorber temperature profiles
  - Midsection scattered (10^{o}C)
  - Top+bottom high reproducibility (1-5^{o}C)



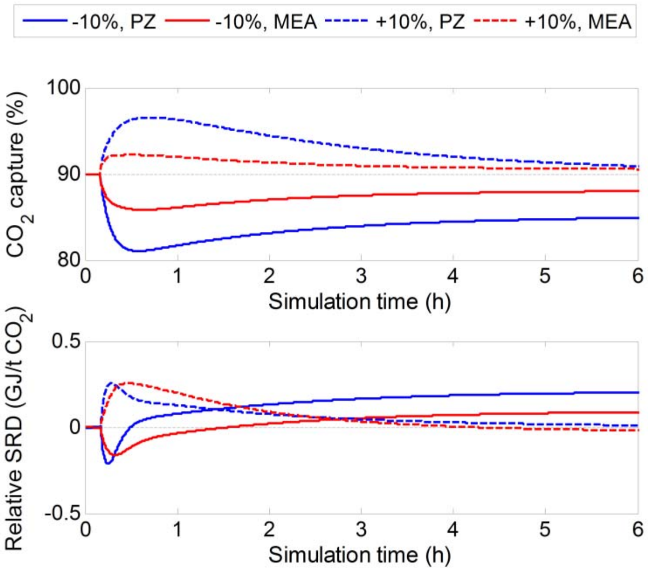
Dynamic Absorber and Desorber Model

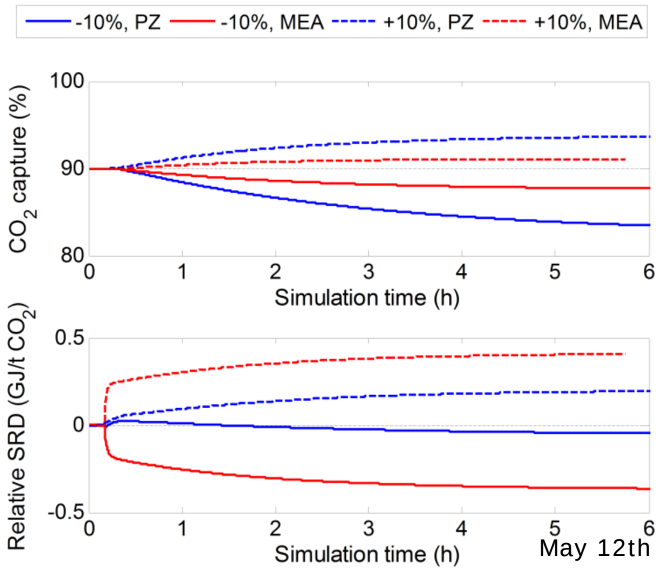
MEA





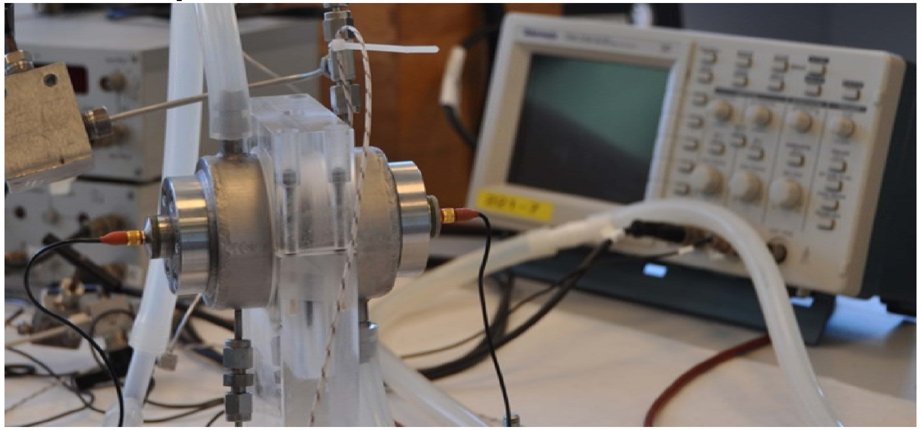
PZ



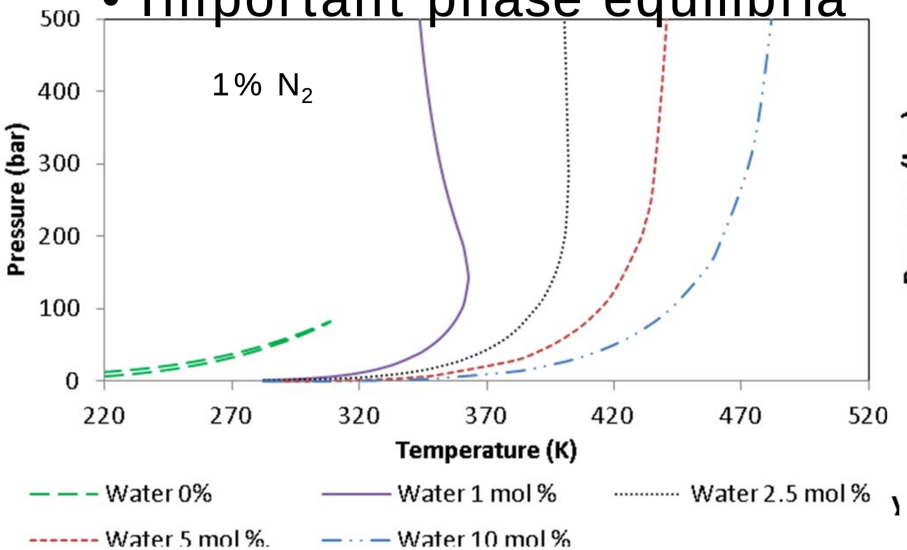


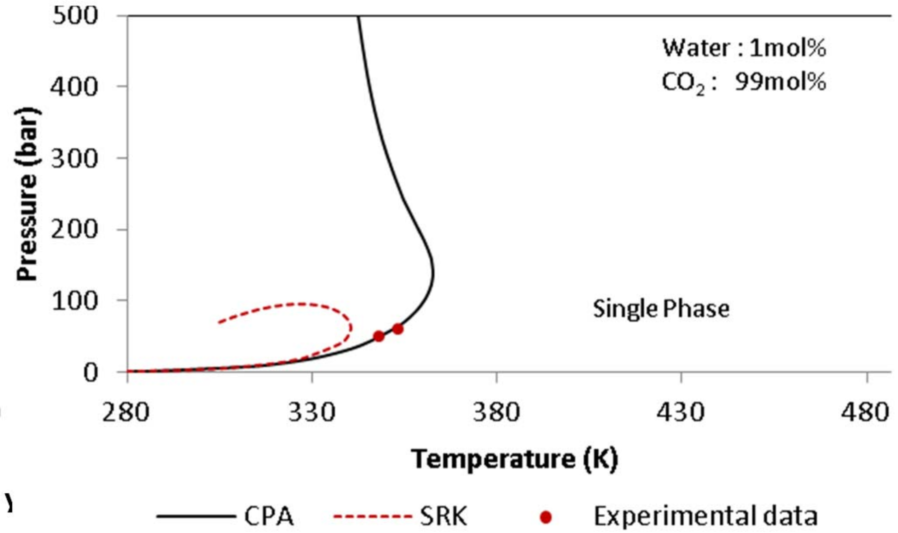
Compression & transport

- Speed of sound
- HP Gas diffusion



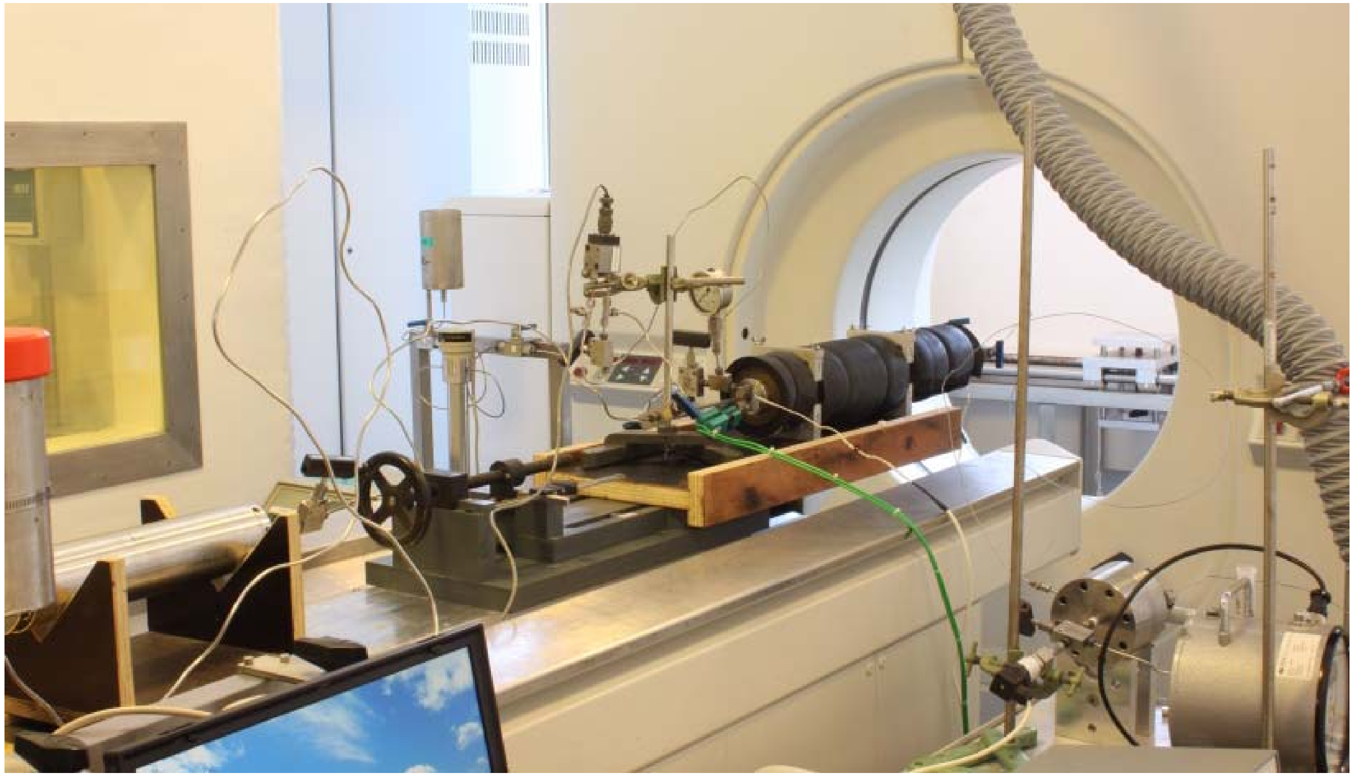
- Important phase equilibria



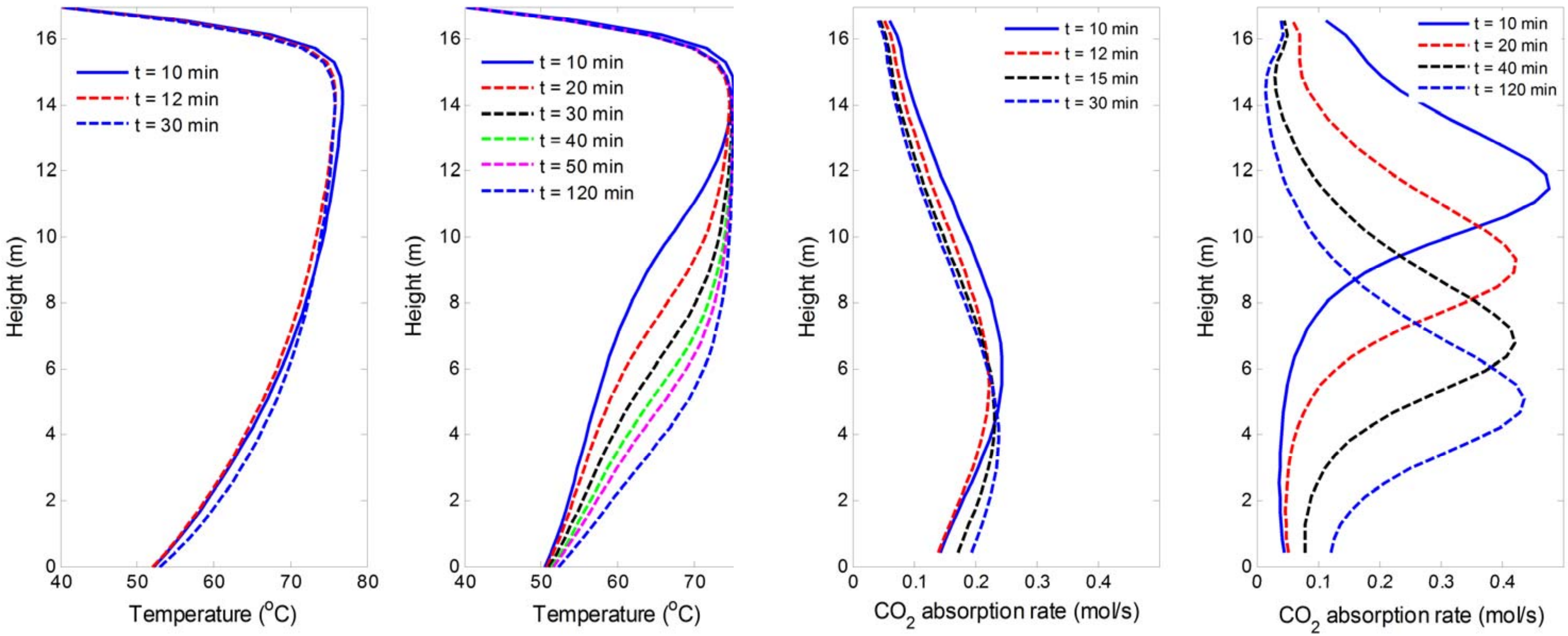


CO_2 storage

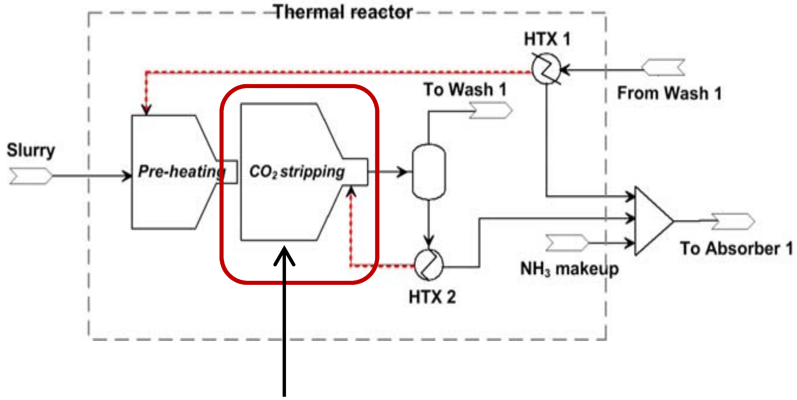
- Reservoir CO_2 injection using CT-scanning



Dynamics (dCapCO2), MEA vs. PZ



Optimization of energy consumption



T = 88 ° C
P = 1 bar

Low- and mid- temperature waste/process heat integration!

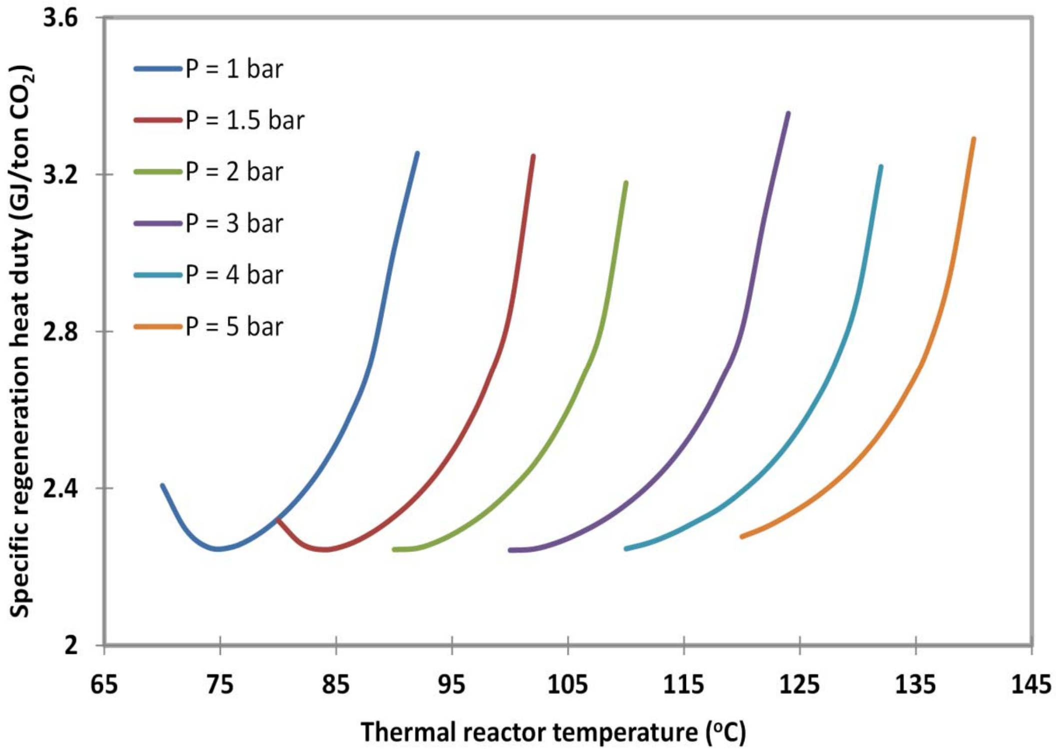


Fig. 5. Influence of temperature and pressure on the specific regeneration energy

Statements on CO_2 emitting energy sources

- Cheap energy sources will be used by 3rd world countries as long as they are available
- Coal and oil are cheap and “easy” energy resources
- Renewable technologies will be beneficial for developed countries but will take longer to implement in the 3rd world
- Several industrial processes produce noticeable amounts of CO_2 which may not be reduced by renewable energy
  - Cement industry
  - Fermentation industry (Medicine, food, and bioethanol production)
  - Agriculture
  - Transportation

CAPCO2 unit operation

Aspen Plus